

TabPFN

GPR

GPT-SMILES

GPT-InChI

GPT-SELFIES

GPT-Name

accuracy

0.50

0.25

0

50

100

150

200

F₁ macro

0.50

0.25

0

50

100

150

200

F₁ micro

0.50

0.25

0

50

100

150

200

κ

0.5

0.0

0

50

100

150

200

number of training points

